AD-A121 415 THEORETICAL PROBLEMS OF THE SOLID STATE(U) CALIFORNIA
UNIV SAN DIEGO LA JOLLA DEPT OF PHYSICS W KOHN NOV 82
N00014-76-C-0050

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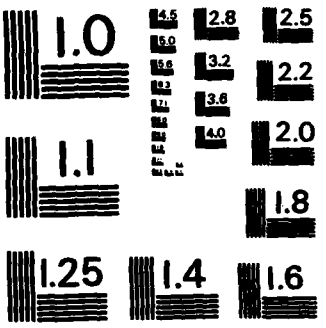

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Final Report

Theoretical Problems of the Solid State

N00014-76-C-0050

1 August 1975 - 30 April 1982

The following work was accomplished under this contract:

1. Contributions to the Electronic theory of surfaces, interfaces and adsorbed storms on surfaces.
   Technical reports 34, 36, 39, 41, 42, 43, 44, 45, 51.
2. Contribution to the Theory of the electronic structure of liquid metals.
   Technical report 35.
3. Local theory of electronic structure of extended systems.
   Technical reports 38, 46.
4. Positron interactions with surfaces.
   Technical reports 48, 49, 50.
5. Combination of Landau-and Density Functional Theory.
   Technical report 52.
6. Theory of fluctuating valence solids.
   Technical reports 53, 54, 55.

In the following paragraphs ~~we describe in greater detail~~ are described: work done during the last renewal period of the above contract, 11/1/79 - 4/30/82.

~~A.~~ A Universal Model for Surface Energies:[1]

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1. Technical report 51.

Surface energy of a solid may be regarded as the reversible work done in clearing and thus creating new surface area. The clearing force, in the initial stage, can be expressed in terms of elastic characteristics (more precisely the phonon spectrum) of the bulk solid; in the final stage (2 new surfaces separated by $\geq 3\mathring{A}$) it can be expressed as a Van-der-Waals like polarization force. A numerical interpolation between these 2 limits can be made. This leads to the result

$$\sigma = \alpha^*(AC)^{1/2}$$

where σ is the surface energy per unit area, A is explicitly given by the bulk-phonon spectrum $\omega(\underset{\sim}{k})$ and C is explicitly given by the bulk dielectric constant $\varepsilon(\omega)$. α^* is a universal dimensionless constant. The value $\alpha^* = 0.48$ gives agreement with experimental results to about $\pm$ 15% for a wide variety of metals.

This "universalist" approach to surface energy has apparently stimulated similar universal proposals for several important physical quantities, such as cohesive and adhesive energies.

B.) Positron Scattering from Surfaces;[2]

This work constituted the thesis of J. Oliva, which emphasizes positronium formation. It deals with four distinct processes. a) The positron enters the metal and is thermalized at a distance of the order of $10^3\mathring{A}$. b) It then undergoes thermal diffusion. c) When reaching the surface again (with probability $\sim$1) it is generally reflected back into the metal. d) Eventually

2. Technical reports 48, 49, 50.

when reaching the surface after several reflections it escapes, generally picking up an electron in the process. Positron scattering has now become an important junior partner to electron scattering for the study of solid surfaces.

C. Narrowing of Hole Bands of Valence Electron Scattering;

This work constituted the thesis of D. Heim. Holes in occupied bands of metals (e.g. the d-band of Zn) are surrounded by a screening band of conduction electrons. This leads to a narrowing of the hole band and to a change of its shape. These calculations have a direct bearing on photoemission experiments. The problem was studied by re-normalization, moment and numerical techniques. A technical report will be prepared.

D. Dynamics Response of Inhomogeneous Fermion Systems; AND

We have developed a theory which combines the Landau theory of Fermi liquids with the Hohenberg-Kohn density functional theory to provide an electric response theory for weakly inhomogeneous electronic systems.

E. Valence Fluctuation Compounds.

We have made several contributions to the theory of fluctuating valence compounds. a) We have developed a theory to explain the motive of the characteristic first order phase transition of these systems. b) We have clarified the nature of the valence fluctuations at zero temperature. c) We have given an explanation of the extended X-ray fine structure (EXAFS) in a mixed valence solid.

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3. D. Heim, Thesis, UC San Diego, 1982.
4. Technical reports 53, 54, 55.
5. Technical reports 53, 54, 55.

LIST OF TECHNICAL REPORTS FOR
CONTRACT NO. N 00014-76-C-0050
1 August 1975 - 30 April 1982

(The report numbers begin with No. 34 following reports Nos. 1-33 associated with a previous contract N 00014-69-A-0200-6026)

No. 34 E. Zaremba, Polarization Induced Surface Dipole Moments

No. 35 J.J. Olson, KKR Analysis of the Anderson-McMillan Theory of Electronic Structure of Liquid Metals

No. 36 E. Zaremba and W. Kohn, Theory of Helium Adsorption on Simple and Noble Metal Surfaces

No. 37 K.H. Lau and W. Kohn, Elastic Interaction of Two Atoms Adsorbed on a Solid Surface

No. 38 J.R. Onffroy, Theory of Shallow Donor States with a Strong Central Cell Perturbation

No. 39 A. Yaniv, Green's Funciton Calculation of a Metal-Metal Interface

No. 40 K.H. Lau and W. Kohn, Oscillatory Indirect Interaction Between Adsorbed Atoms

No. 41 C.C. Pei, Perturbation of Electronic Structure of Insulators by Interfaces and Defect

No. 42 A. Yaniv, The Electronic Properties of a Simple Metal-Metal Interface

No. 43 C.C. Pei, Interface Energies

No. 44 O. Hipolito, Binding Energy and Effective Mass of Charged Particles Trapped on Surfaces

No. 45 R.K. Kalia and P. Vashishta, Surface Structure of Electron-Hole Drops in Germanium and Silicon

No. 46 A. Yaniv and W. Kohn, Local Theory of Electronic Structure of Extended Systems

No. 47 A. Yaniv and W. Kohn, Locality Principle in Wave-Mechanics

No. 48 J. Oliva, Quasiparticle Damping of a Positron in an Electron Gas

No. 49 J. Oliva, New Calculational Scheme for Particle Range and an Application to a Positron Entering a Metal

No. 50 J. Oliva, Physical Processes in Positronium Formulation at Metal Surfaces

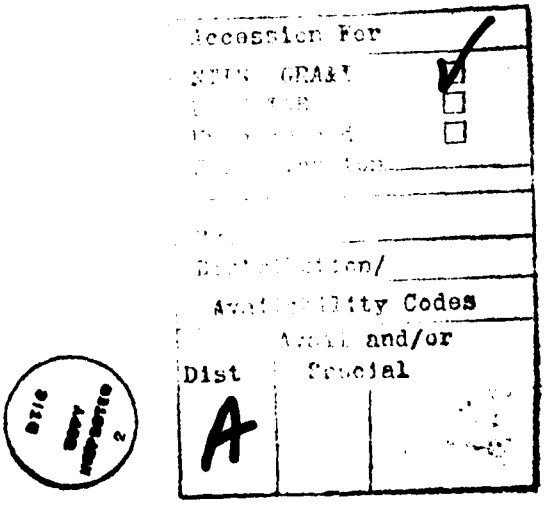
No. 51 W. Kohn and A. Yaniv, Universal Model for the Surface Energy of Solids

No. 52 S. Chakravarty et al, Dynamic Response of Inhomogeneous Fermi Systems

No. 53 L. Falicov et al, First-Order Phase Transitions in Intermediate Valence Solids--a Theory Based on Metallic Hydrogen

No. 54 W. Kohn and T.K. Lee, Fluctuation Effects in Mixed Valence Systems at Zero Temperature

No. 55 W. Kohn et al, Theory of Extended X-Ray Absorption Fine Structure (EXAFS) in a Mixed Valence Solid



LIST OF PUBLICATIONS FOR

CONTRACT NO. N 00014-76-C-0050

1 August 1975 - 30 April 1982

1. J.J. Olson, Anderson-McMillan Theory of Electronic Structure of Liquid Metals, Phys. Rev. B12, 2908 (1975).

2. K.H. Lau and W. Kohn, Non-Local Corrections to the Electronic Structure of Metal Surfaces, J. Phys. Chem. Solids 37, 99 (1976).

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5. K.H. Lau and W. Kohn, Adatom Dipole Moments on Metals and Their Interactions, Solid State Commun. 18, 553 (1976).

6. W. Kohn, Theory of Helium Adsorption on Simple and Noble Metal Surfaces, Phys. Rev. B15, 1769 (1977).

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8. A. Yaniv and W. Kohn, Locality Principle in Wave-Mechanics, Proc. Nat. Acad. Sci., USA 75, No. 11, 5270 (1978).

9. R.K. Kalia and P. Vashishta, Surface Structure of Electron-Hole Drops in Germanium and Silicon, Phys. Rev. B17, 2655 (1978).

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11. A. Yaniv and W. Kohn, Universal Model for the Surface Energy of Solids, Phys. Rev. 20, No. 12, 4949 (1979).

12. S. Chakravarty et al, Dynamic Response of Inhomogeneous Fermi Systems, Phys. Rev. Lett. 43, 775 (1979).

13. A. Yaniv and W. Kohn, Local Theory of Electronic Structure of Extended Systems, Festschrift for Felix Bloch, Rice University Studies, Vol. 66, No. 3, 99 (1980).

14. J. Oliva, Inelastic Positron Scattering in an Electron Gas, Phys. Rev. B21, 4909 (1980).

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16. J. Oliva, Physical Processes in Positronium Formulation at Metal Surfaces, Phys. Rev. B21, 4925 (1980).

17. P. Vashishta and W. Kohn, General Density Function Theory, (to be published as a chapter of "The Inhomogeneous Electron Gas," S. Lundqvist and N.H. March, eds.).

18. T.K. Lee and W. Kohn, Fluctuation Effects in Mixed Valence Systems at Zero Temperature, Phil. Mag. A 45, 313 (1982).

19. L.M. Falicov et al, First-Order Phase Transitions in Intermediate Valence Solids--a Theory Based on Metallic Hydrogen, Phys. Rev. B24, 5664 (1981).

20. W. Kohn et al, Theory of Extended X-Ray Absorption Fine Structure (EXAFS) in a Mixed Valence Solid, Phys. Rev. B25, 3557 (1982).